

(FILE 'HOME' ENTERED AT 14:31:57 ON 15 NOV 2003)

FILE 'REGISTRY' ENTERED AT 14:32:11 ON 15 NOV 2003

L1 STRUCTURE UPLOADED
L2 3 S L1 SSS SAM
L3 2200 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 2 S L4 SSS SAM
L6 1269 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 0 S L7 SSS SAM
L9 6 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:41:33 ON 15 NOV 2003

FILE 'CAPLUS, USPATFULL' ENTERED AT 14:41:42 ON 15 NOV 2003

L10 5 S L9

FILE 'REGISTRY' ENTERED AT 14:46:43 ON 15 NOV 2003

L11 STRUCTURE UPLOADED
L12 1 S L11 SSS SAM
L13 35 S L11 SSS FULL

FILE 'CAPLUS, USPATFULL' ENTERED AT 14:47:40 ON 15 NOV 2003

L14 15 S L13

=> d 114 1-15 ibib abs hitstr

L14 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:719208 CAPLUS

DOCUMENT NUMBER: 136:53590

TITLE: Design, Synthesis, and Characterization of the

Antitumor Activity of Novel Ceramide Analogues

AUTHOR(S): Macchia, Marco; Barontini, Silvia; Bertini, Simone; Di
Bussolo, Valeria; Fogli, Stefano; Giovannetti, Elisa;

Grossi, Enzo; Minutolo, Filippo; Danesi, Romano

CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of
Pisa, Pisa, 56126, Italy

SOURCE: Journal of Medicinal Chemistry (2001), 44(23),
3994-4000

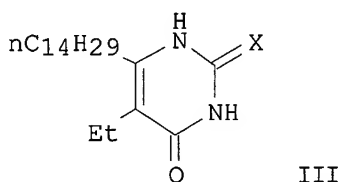
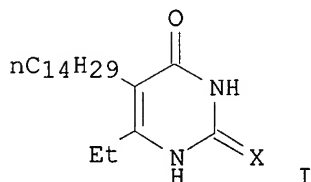
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



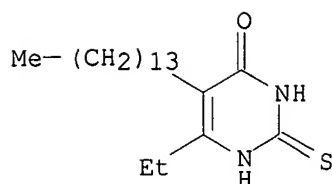
AB A deficiency in apoptosis is one of the key events in the proliferation and resistance of malignant cells to antitumor agents; for these reasons, the search for apoptosis-inducing drugs represents a valuable approach for the development of novel anticancer therapies. In this study we report the first example of conformationally restrained analogs of ceramide, where the polar portion of the mol. has been replaced by a thiouracil {[I; X = S (II)], [III; X = S (IV)]} or uracil I [X = O (V)], III [X = O (VI)] ring. The evaluation of their biol. activity on CCRF-CEM human leukemia cells demonstrated that the most active was II followed by V (mean 50% inhibition of cell proliferation [IC50] 1.7 and 7.9 .mu.M, resp.), while compds. IV and VI were inactive, as were uracil, thiouracil, and 5,6-dimethyluracil, the pyrimidine moieties of compds. II, IV-VI. For comparison, the IC50 of the ref. substance, the cell-permeable C2-ceramide, was 31.6 .mu.M. Compds. II and V and C2-ceramide were able to trigger apoptosis, as shown by the occurrence of DNA and nuclear fragmentation, and to release cytochrome c from treated cells. The treatment of female CD-1 nu/nu athymic mice bearing a WiDr human colon xenograft with the most active compd. II at 2, 10, 50, and 200 mg/kg i.p. daily for 10 days resulted in an antitumor effect that was equiv. at 50 mg/kg or superior (200 mg/kg) to that of cyclophosphamide, 20 mg/kg i.p. daily, delivered on the same schedule, with markedly lower systemic toxicity. In conclusion, the present study demonstrates that the new ceramide analogs II and V are characterized by in vitro and in vivo antitumor activity and low toxicity.

IT 322391-32-2P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and antitumor activity of ceramide analogs)

RN 322391-32-2 CAPLUS

CN 4(1H)-Pyrimidinone, 6-ethyl-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



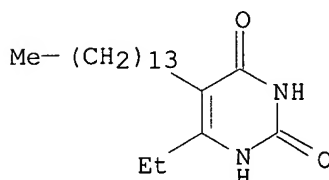
IT 322391-33-3P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and antitumor activity of ceramide analogs)

RN 322391-33-3 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-ethyl-5-tetradecyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:78368 CAPLUS

DOCUMENT NUMBER: 134:131369

TITLE: process for the preparation of ceramide analogs and their use as antitumor agents

INVENTOR(S): Macchia, Bruno; Balsamo, Aldo; Macchia, Marco; Del Tacca, Mario; Danesi, Romano

PATENT ASSIGNEE(S): Bracco S.p.A., Italy

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

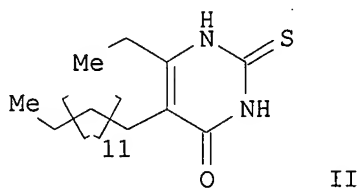
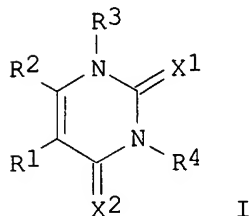
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

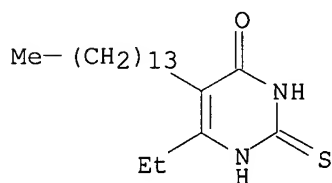
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007418	A2	20010201	WO 2000-EP7023	20000721
WO 2001007418	A3	20010510		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
IT 1307786	B1	20011119	IT 1999-FI169	19990722
EP 1198458	A2	20020424	EP 2000-956250	20000721
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			

JP 2003505451 T2 20030212 JP 2001-512504 20000721
 PRIORITY APPLN. INFO.: IT 1999-FI169 A 19990722
 WO 2000-EP7023 W 20000721
 OTHER SOURCE(S): MARPAT 134:131369
 GI



AB The present invention discloses a process for the prepn. of ceramide analog (I; X1, X2 = O, S; R1, R2 = (CH2)13Me, (un)substituted alkyl, (un)substituted alkylene groups with one or more substituents selected among arom., primary, secondary and tertiary aminic, quaternary ammonium, CO2H, OH, polyoxyalkyl and ethereal groups, amino acids, halogen, saccharidic portions, providing that between R1 and R2 only one is (CH2)13Me; R3, R4 = H, (un)substituted alkyl, (un)substituted alkylene groups with one or more substituents selected among arom., primary, secondary and tertiary aminic, quaternary ammonium, CO2H, OH, polyoxyalkyl and ethereal groups, amino acids, halogen, saccharidic portion) and pharmaceutical formulations for the treatment of tumors. Thus, II was prepd. by the reaction of .beta.-ketoester III, Me(CH2)14CH(COCH2Me)COOCH2Me (obtained by the reaction of Et palmitate and propionyl chloride), with thiourea. II shows IC50 of 1.7 .mu.M in tests against human leukemia cell line called CCRF/CEM.

IT 322391-32-2P
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (process for the prepn. of ceramide analogs and their use as antitumor agents)
 RN 322391-32-2 CAPLUS
 CN 4(1H)-Pyrimidinone, 6-ethyl-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



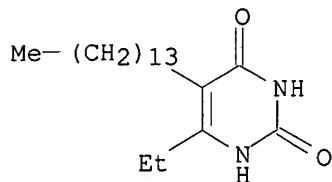
IT 322391-33-3P 322391-34-4P 322391-35-5P
 322391-36-6P 322391-37-7P 322391-38-8P
 322391-39-9P 322391-40-2P 322391-41-3P
 322391-42-4P 322391-43-5P 322391-44-6P
 322391-48-0P 322391-51-5P 322391-52-6P
 322391-54-8P 322391-55-9P 322391-56-0P
 322391-57-1P
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

PREP (Preparation); USES (Uses)

(process for the prepn. of ceramide analogs and their use as antitumor agents)

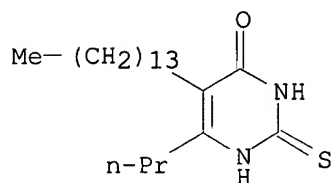
RN 322391-33-3 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-ethyl-5-tetradecyl- (9CI) (CA INDEX NAME)



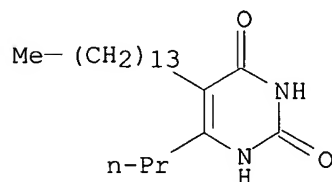
RN 322391-34-4 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-propyl-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



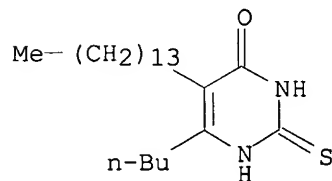
RN 322391-35-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-propyl-5-tetradecyl- (9CI) (CA INDEX NAME)



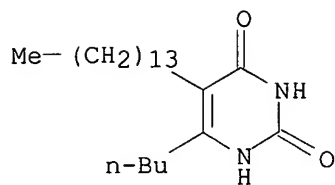
RN 322391-36-6 CAPLUS

CN 4(1H)-Pyrimidinone, 6-butyl-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



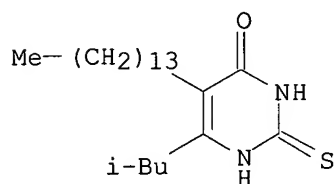
RN 322391-37-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-butyl-5-tetradecyl- (9CI) (CA INDEX NAME)



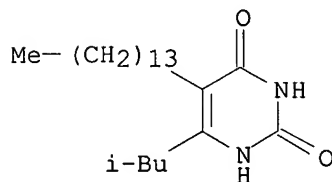
RN 322391-38-8 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-(2-methylpropyl)-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



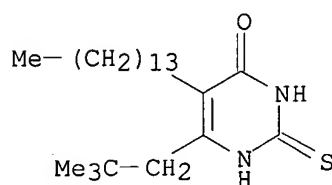
RN 322391-39-9 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-(2-methylpropyl)-5-tetradecyl- (9CI) (CA INDEX NAME)



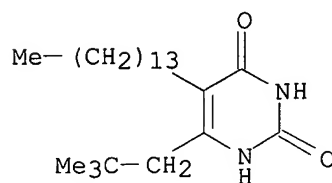
RN 322391-40-2 CAPLUS

CN 4(1H)-Pyrimidinone, 6-(2,2-dimethylpropyl)-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)

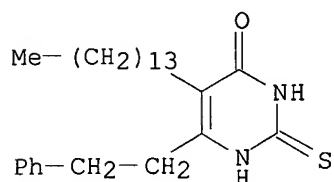


RN 322391-41-3 CAPLUS

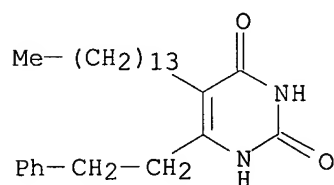
CN 2,4(1H,3H)-Pyrimidinedione, 6-(2,2-dimethylpropyl)-5-tetradecyl- (9CI) (CA INDEX NAME)



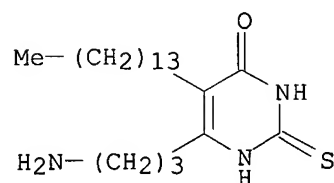
RN 322391-42-4 CAPLUS
 CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-(2-phenylethyl)-5-tetradecyl-2-thio-
 (9CI) (CA INDEX NAME)



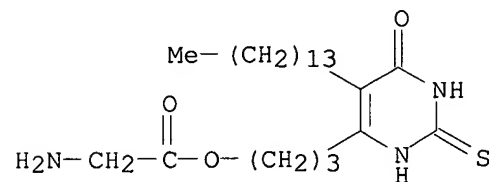
RN 322391-43-5 CAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 6-(2-phenylethyl)-5-tetradecyl- (9CI) (CA
 INDEX NAME)



RN 322391-44-6 CAPLUS
 CN 4(1H)-Pyrimidinone, 6-(3-aminopropyl)-2,3-dihydro-5-tetradecyl-2-thio-
 (9CI) (CA INDEX NAME)

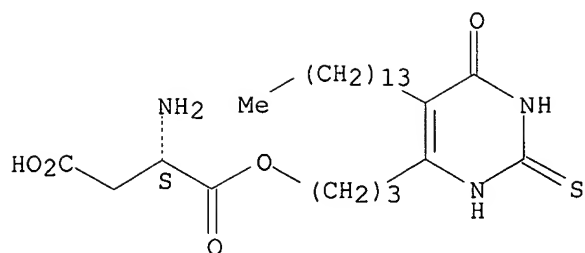


RN 322391-48-0 CAPLUS
 CN Glycine, 3-(1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thio-4-
 pyrimidinyl)propyl ester (9CI) (CA INDEX NAME)



RN 322391-51-5 CAPLUS
 CN L-Aspartic acid, 1-[3-(1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thio-4-
 pyrimidinyl)propyl] ester (9CI) (CA INDEX NAME)

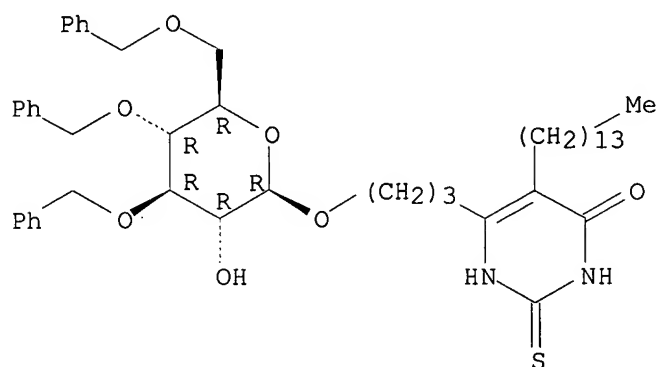
Absolute stereochemistry.



RN 322391-52-6 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-5-tetradecyl-2-thioxo-6-[3-[[3,4,6-tris-O-(phenylmethyl)-.beta.-D-glucopyranosyl]oxy]propyl]- (9CI) (CA INDEX NAME)

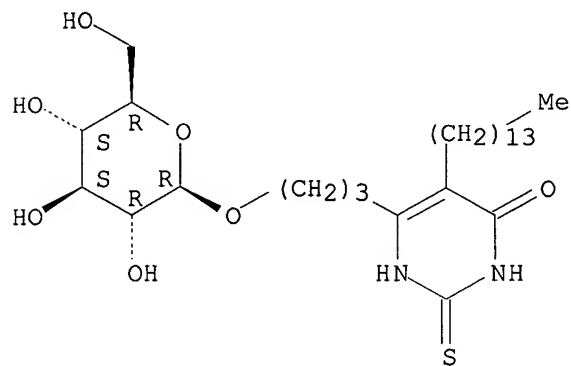
Absolute stereochemistry.



RN 322391-54-8 CAPLUS

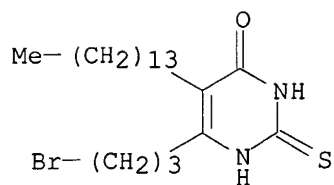
CN 4(1H)-Pyrimidinone, 6-[3-(.beta.-D-glucopyranosyloxy)propyl]-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



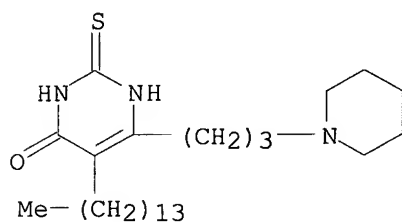
RN 322391-55-9 CAPLUS

CN 4(1H)-Pyrimidinone, 6-(3-bromopropyl)-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



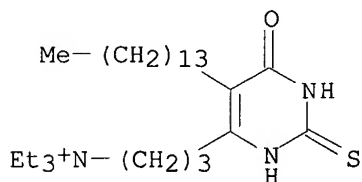
RN 322391-56-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-[3-(1-piperidinyl)propyl]-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 322391-57-1 CAPLUS

CN 4-Pyrimidinepropanaminium, N,N,N-triethyl-1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thioxo-, bromide (9CI) (CA INDEX NAME)



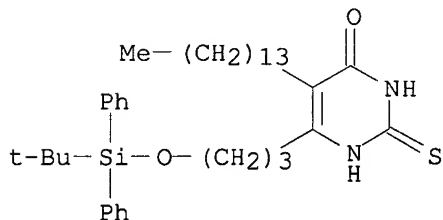
● Br⁻

IT 322391-45-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the prepn. of ceramide analogs and their use as antitumor agents)

RN 322391-45-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[3-[[1,1-dimethylethyl)diphenylsilyl]oxy]propyl]-2,3-dihydro-5-tetradecyl-2-thioxo- (9CI) (CA INDEX NAME)



IT 322391-46-8P 322391-47-9P 322391-49-1P

322391-50-4P

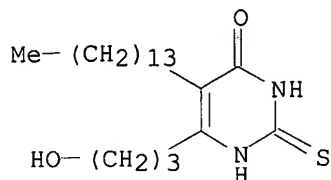
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(process for the prepn. of ceramide analogs and their use as antitumor agents)

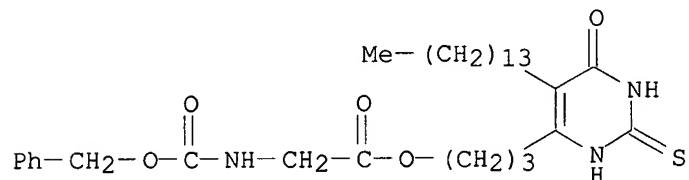
RN 322391-46-8 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-(3-hydroxypropyl)-5-tetradecyl-2-thioxo-
(9CI) (CA INDEX NAME)



RN 322391-47-9 CAPLUS

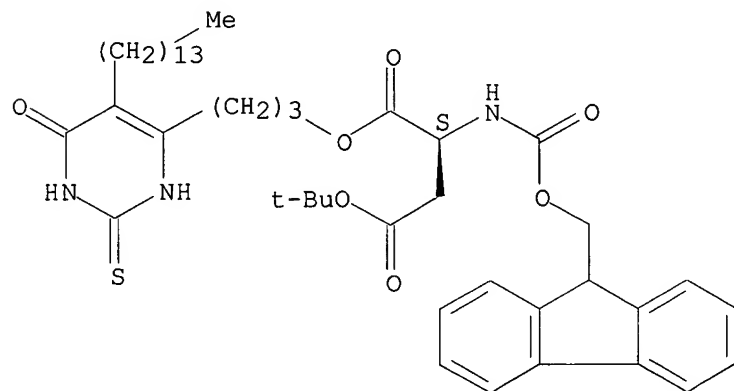
CN Glycine, N-[(phenylmethoxy)carbonyl]-, 3-(1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thioxo-4-pyrimidinyl)propyl ester (9CI) (CA INDEX NAME)



RN 322391-49-1 CAPLUS

CN L-Aspartic acid, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-, 4-(1,1-dimethylethyl) 1-[3-(1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thioxo-4-pyrimidinyl)propyl] ester (9CI) (CA INDEX NAME)

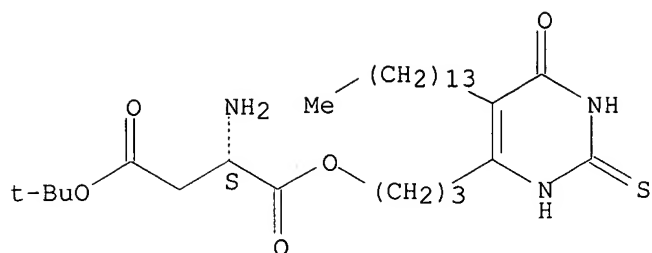
Absolute stereochemistry.



RN 322391-50-4 CAPLUS

CN L-Aspartic acid, 4-(1,1-dimethylethyl) 1-[3-(1,2,3,6-tetrahydro-6-oxo-5-tetradecyl-2-thioxo-4-pyrimidinyl)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:504915 CAPLUS

DOCUMENT NUMBER: 123:55797

TITLE: Preparation, characterization, and antimicrobial activity of some 5-alkyl-2,4,6-substituted pyrimidines

AUTHOR(S): Koos, M.; Novotna, Z.

CORPORATE SOURCE: Inst. Chemistry, Slovak Acad. Sci., Bratislava, SK-842 38, Slovakia

SOURCE: Chemical Papers (1994), 48(4), 278-81

CODEN: CHPAEG; ISSN: 0366-6352

PUBLISHER: Slovak Academy of Sciences, Institute of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

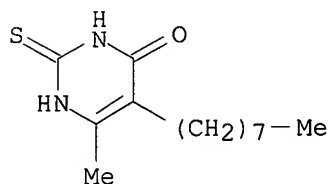
AB Fifteen new 5-alkyl-2,4,6-substituted pyrimidines were prepd. by cyclization of alkylmalononitriles, Et 2-cyanoalkanoates, or 2-alkyl-3-oxobutyrate. Spectral data as well as values of min. inhibitory concn. against selected microorganisms are given. No significant antimicrobial efficiency was found.

IT 59224-18-9P 164530-38-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antimicrobial activity of some alkylpyrimidines)

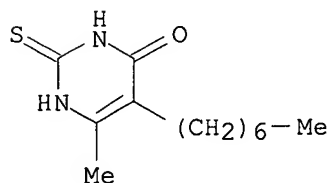
RN 59224-18-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA INDEX NAME)

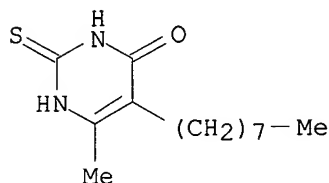


RN 164530-38-5 CAPLUS

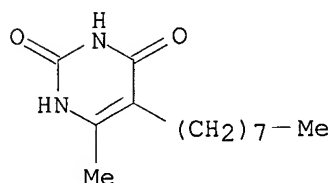
CN 4(1H)-Pyrimidinone, 5-heptyl-2,3-dihydro-6-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L14 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1994:457445 CAPLUS
 DOCUMENT NUMBER: 121:57445
 TITLE: Oxidation of substituted 2-thiouracils and
 pyrimidine-2-thione with ozone and
 3,3-dimethyl-1,2-dioxirane
 AUTHOR(S): Claudia, Crestini; Mincione, Enrico; Saladino,
 Raffaele; Nicoletti, Rosario
 CORPORATE SOURCE: Dip. Chim., Univ. Roma "La Sapienza", Rome, 00185,
 Italy
 SOURCE: Tetrahedron (1994), 50(10) 3259-72
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ozone and 3,3-dimethyl-1,2-dioxirane react with substituted 2-thiouracils
 and pyrimidine-2-thione to afford several desulfurized products. The
 effect of the solvent, protic as opposed to nonprotic, on the course of
 oxidn. was striking.
 IT 59224-18-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidn. of, with ozone)
 RN 59224-18-9 CAPLUS
 CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA
 INDEX NAME)



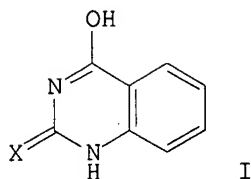
IT 94815-69-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 94815-69-7 CAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 6-methyl-5-octyl- (9CI) (CA INDEX NAME)



L14 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1993:428095 CAPLUS
 DOCUMENT NUMBER: 119:28095
 TITLE: Ozonation of substituted 2-thiouracils and
 pyrimidine-2-thione
 AUTHOR(S): Crestini, Claudia; Saladino, Raffaele; Nicoletti,
 Rosario
 CORPORATE SOURCE: Dip. Chim., Univ. Roma La Sapienza, Rome, 00100, Italy
 SOURCE: Tetrahedron Letters (1993), 34(10), 1631-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

OTHER SOURCE(S):
GI

CASREACT 119:28095



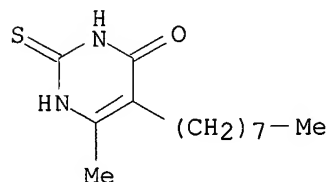
AB The ozonation of substituted 2-thiouracils and pyrimidine-2-thione, e.g., I (X = S) is reported; this provides a new method for the synthesis of several pyrimidine derivs. E.g., I (X = S) underwent ozonation in acetic acid-water to give quinazolidione I (X = O) in 75%. I (X = S) underwent ozonation in acetic acid alone to give quinazolinone I (X = H) in 82%.

IT **59224-18-9**

RL: PROC (Process)
(ozonation of)

RN 59224-18-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA INDEX NAME)

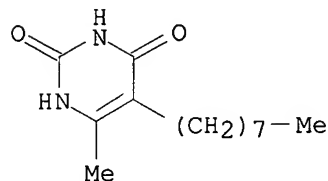


IT **94815-69-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 94815-69-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-methyl-5-octyl- (9CI) (CA INDEX NAME)



L14 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:101984 CAPLUS

DOCUMENT NUMBER: 118:101984

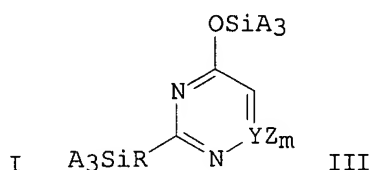
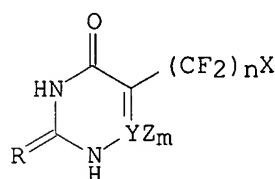
TITLE: Preparation of fluoroalkyl group-containing pyrimidine derivatives as intermediates for carcinostatics and virucides

INVENTOR(S): Nishida, Masakazu; Fujii, Shozo; Kimoto, Hiroshi;
Hayakawa, Yoshio; Sawada, Hideo; Mitani, Motohiro;
Nakayama, Masaharu

PATENT ASSIGNEE(S): Agency of Industrial Sciences and Technology, Japan;
Nippon Oil and Fats Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04261161	A2	19920917	JP 1991-20901	19910214
JP 3032837	B2	20000417		

PRIORITY APPLN. INFO.: JP 1991-20901 19910214
OTHER SOURCE(S): CASREACT 118:101984; MARPAT 118:101984
GI



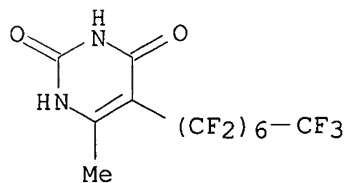
AB The title derivs. I (R = O, S; X = H, F, Cl; Y = C, N; Z = H, CF3, C1-4 alkyl; m = 0, 1; n = 1-10; when Y = C then m = 1; when Y = N then m = 0) are prep'd. by treating X(CF2)nCO2OCO(CF2)nX (II) with pyrimidines III (A = C1-4 alkyl). Treating 6-methyluracil in dioxane with Et3N and ClSiMe3 gave quant. III (A = Z = Me, R = O, Y = C), a soln. of which in CF2ClCFC12 was treated dropwise with a soln. of II (X = F, n = 3) in CF2ClCFC12 at 30.degree., stirred at the same temp. for 2 h, then refluxed for 1.5 h to give 36% I.

IT 145663-06-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as carcinostatic and virucide)

RN 145663-06-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-methyl-5-(pentadecafluoroheptyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:78816 CAPLUS

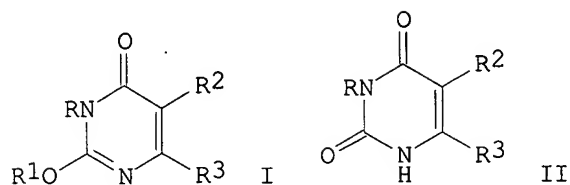
DOCUMENT NUMBER: 102:78816

TITLE: 6-Alkyl and 5,6-dialkyl-2-methoxy-4(3H)-pyrimidinones in the transformations of pyrimidines - 2. Synthesis and conversion into alkyluracils and 2-alkoxy-4(3H)-pyrimidinones

AUTHOR(S): Botta, M.; Cavalieri, M.; Ceci, D.; De Angelis, F.; Finizia, G.; Nicoletti, R.

CORPORATE SOURCE: Dep. Chem., Univ. "La Sapienza", Rome, 00185, Italy

SOURCE: Tetrahedron (1984), 40(17), 3313-20
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 102:78816
 GI



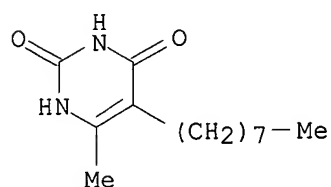
AB Alkoxyppyrimidinones I [R = H; R1 = Me; R2 = H, R3 = Me, Et; R2 = R3 = Me; R2R3 = (CH2)4] were obtained by treating R3COCHR2CO2Et with MeOC(NH2):NH.H2SO4 and Ca(OH)2. Similar reaction, followed by acidification, gave pyrimidinediones II [R = H; R2 = H, Me, allyl, octyl; R3 = Me, Et, pentyl, cyclohexyl; R2R3 = (CH2)4]. I (R1 = Et, Bu, cyclohexyl) were prepd. by transalkylation of I (R1 = Me) with alcoholate. I (R = H, R1 = Me) and II (R = H) were N-methylated with Me2SO4 to give I and II (R = Me).

IT 94815-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 94815-69-7 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-methyl-5-octyl- (9CI) (CA INDEX NAME)



L14 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:400355 CAPLUS

DOCUMENT NUMBER: 85:355

TITLE: Antiviral compounds. X. Synthesis and anti-influenza virus activity of 2-substituted 5-alkyl-6-hydroxy-4-methylpyrimidines

AUTHOR(S): Nishimura, Tamio; Miyamoto, Yoshiko; Fukuyasu, Harumi

CORPORATE SOURCE: Sch. Hyg. Sci., Kitasato Univ., Sagamihara, Japan

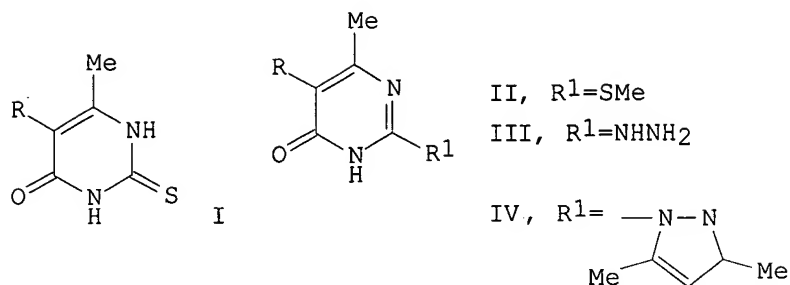
SOURCE: Yakugaku Zasshi (1976), 96(3), 384-7

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



R: a=Me, b=Pr, c=(CH₂)₅Me, d=(CH₂)₇Me, e=(CH₂)₉Me

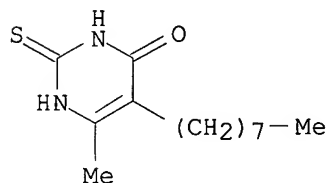
AB 2-Mercapto-(I), 2-methylthio-(II), 2-hydrazino-(III), and 2-(3,5-dimethyl-1-pyrazolyl)-5-alkyl-6-hydroxypyrimidines (IV) were synthesized and their antiinfluenza virus activity was examd. Among the tested compds., viral inhibitory activity was obsd. with IVb [59224-16-7] (50% inhibitory concn. = 4.7 .mu.g/ml) and IVc [59224-17-8] (339 .mu.g/ml). However, almost all the compds. exhibited a virucidal activity, esp. Id [59224-18-9] (50% virucidal condn. = 90 .mu.g/ml) and IIIc [59224-19-0] (130 .mu.g/ml). Compds. which showed toxic concn. of more than 125 .mu.g/ml against HeLa cells were tested in infected mice. When administered at 100 mg/kg, i.p., Ie [59224-20-3], IIa [54855-79-7], and IIb [59144-22-8] showed 71, 62, and 62% inhibition of the virus multiplication in the lungs, resp. However; Ie was inactive when administered orally.

IT 59224-18-9 59224-20-3

RL: BIOL (Biological study)
 (influenza virus inhibition by)

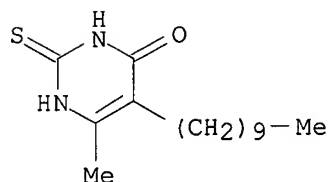
RN 59224-18-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA INDEX NAME)

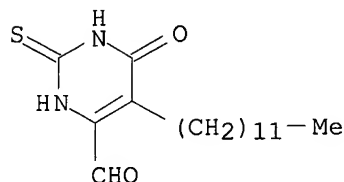


RN 59224-20-3 CAPLUS

CN 4(1H)-Pyrimidinone, 5-decyl-2,3-dihydro-6-methyl-2-thioxo- (9CI) (CA INDEX NAME)



DOCUMENT NUMBER: 76:137435
 TITLE: Inhibition of thymidylc acid kinase by 5-substituted pyrimidines
 AUTHOR(S): Chae, Chi-Bom; Dobbins, M. Catherine; Irvin, J. Logan; Piantadosi, Claude
 CORPORATE SOURCE: Dep. Biochem., Univ. North Carolina, Chapel Hill, NC, USA
 SOURCE: Biochemical Pharmacology (1972), 21(6), 761-70
 CODEN: BCPA6; ISSN: 0006-2952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB -Mercapto-5-(p-chlorobenzyl)orotic aldehyde (I) inhibits the incorporation of labeled thymidine into TTP and DNA in Ehrlich ascites carcinoma cells in vitro. I inhibits phosphorylation of TMP to TDP by high-speed supernatants of Ehrlich ascites carcinoma and regenerating rat liver, and the inhibition is of the competitive type. I does not affect thymidine kinase, TDP kinase, or the phosphorylation of uridine to UTP in high-speed supernatants of Ehrlich ascites carcinoma. Pyrimidines with bulky groups at the C-5 position inhibit TMP kinase.
 IT 31349-92-5
 RL: BIOL (Biological study)
 (thymidylate kinase inhibition by)
 RN 31349-92-5 CAPLUS
 CN 4-Pyrimidinecarboxaldehyde, 5-dodecyl-1,2,3,6-tetrahydro-6-oxo-2-thioxo- (9CI) (CA INDEX NAME)



L14 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1971:51983 CAPLUS
 DOCUMENT NUMBER: 74:51983
 TITLE: Potential anticancer agents. VI. 5-Substituted pyrimidine-6-carboxaldehydes
 AUTHOR(S): Piantadosi, Claude; Hong, Chung Il; Irvin, J. Logan
 CORPORATE SOURCE: Sch. Med., Univ. North Carolina, Chapel Hill, NC, USA
 SOURCE: Journal of Pharmaceutical Sciences (1970), 59(11), 1637-45
 CODEN: JPMSAE; ISSN: 0022-3549
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB 2-Mercapto-4-hydroxy-5-(3-phenylpropyl)pyrimidine-6-carboxaldehyde (I), 2-mercapto-4-hydroxy-5-(4-phenylbenzyl)-pyrimidine-6-carboxaldehyde (II), 2-mercapto-4-hydroxy-5-(.alpha.-naphthylmethyl)pyrimidine-6-carboxaldehyde, and 14 other 5-substituted pyrimidine-6-carboxaldehydes were synthesized and the 1st 3 compds. were equally as effective as 5-fluorouracil and 2-mercapto-4-hydroxy-5-(4-chlorobenzyl)pyrimidine-6-carboxaldehyde in inhibiting formate incorporation into DNA and growth of Ehrlich ascites tumor cells in vitro. They were more effective than 5-fluorouracil in inhibiting incorporation of formate and orotic acid into RNA, thymidine into DNA, and phenylalanine into proteins. The active compds. strongly inhibited respiration of the ascitic tumor. Also, I and II inhibited growth of Ehrlich carcinoma as a solid tumor after s.c. transplantation, but in these tests the drugs were more toxic to the host

when injected i.p. since the drugs were not preferentially absorbed by the tumor cells in contrast to the tests vs. the ascites form of the carcinoma.

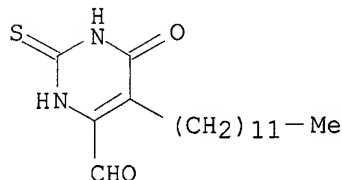
IT **31349-92-5**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(neoplasm inhibition by)

RN 31349-92-5 CAPLUS

CN 4-Pyrimidinecarboxaldehyde, 5-dodecyl-1,2,3,6-tetrahydro-6-oxo-2-thioxo- (9CI) (CA INDEX NAME)

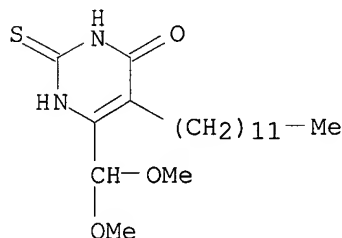


IT **31349-22-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 31349-22-1 CAPLUS

CN Orotaldehyde, 5-dodecyl-2-thio-, 4-dimethyl acetal (8CI) (CA INDEX NAME)



L14 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1963:441710 CAPLUS

DOCUMENT NUMBER: 59:41710

ORIGINAL REFERENCE NO.: 59:7526f-h,7527a

TITLE: Syntheses and antimicrobial activity of
5-alkyl-2-thiouracil derivatives

AUTHOR(S): Watanabe, Sumiko; Tsuji, Tadakazu; Toyoshima, Shigeshi

CORPORATE SOURCE: Keio-Gijukun Univ., Tokyo

SOURCE: Chemical & Pharmaceutical Bulletin (1963), 11, 495-9

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

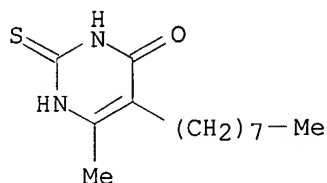
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

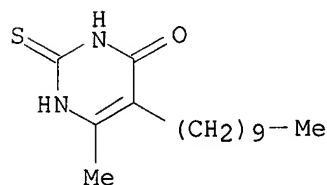
AB In general, 2-thio-5-alkyluracils (I, W = SH, X = H, Z = OH) were prepd. according to a modified method of Anderson (CA 40, 14546). RCO₂Et (0.1 mole) and 0.2 mole HCO₂Et were added during 4 hrs. to 0.13 mole powd. Na in dry ether, the mixt. kept overnight, evapd., and the residue refluxed 7 hrs. on a water bath with 0.08 mole powd. thiourea in abs. EtOH. 2-Thio-5-alkyl-6-methyluracils (I, W = SH, X = Me, Z = OH) (II) were prepd. by condensation of AcCHRCO₂Et with thiourea in EtONa-EtOH according to Russell (CA 46, 2075c). Condensation of RCH(CN)CO₂Et with thiourea gave the 2-thio-5-alkyl-6-aminouracils (I, W = SH, X = H₂N, Z = HO) (III), and these (0.1 mole) refluxed 3-4 hrs. with 0.13 mole MeI and 0.1 mole

EtONa in EtOH gave the 2-methylthio-5-alkyl-6-amino-4-pyrimidinols (I, W = MeS, X = H₂N, Z = HO) (IV), which (0.01 mole) refluxed 5-6 hrs. with 30 cc. POCl₃ gave the 2-methylthio-4-chloro-5-alkyl-6-aminopyrimidines (I, W = MeS, X = H₂N, Z = Cl) (V). The previously unknown compds. thus synthesized were reported (compd., R, m.p. given): I, Bu, 150-1.degree.; I, C₆H₁₃, 171-2.degree.; II, C₆H₁₃, 181-3.degree.; II, C₈H₁₇, 178-80.degree.; II, C₁₀H₂₁, 175-6.degree.; II, C₁₂H₂₅, 170-2.degree.; III, Et, 283-4.degree.; III, Pr, 247-8.degree.; III, Bu, 251-2.degree.; III, C₅H₁₁, 257.degree.; III, C₆H₁₃, 245-6.degree.; IV, Et, 215-17.degree.; IV, Pr, 193-4.degree.; IV, Bu, 170-1.degree.; IV, C₅H₁₁, 167-8.degree.; IV, C₆H₁₃, 165-6.degree.; IV, C₈H₁₇, 160-1.degree.; IV, C₁₀H₂₁, 134-5.degree.; V, Me, 242.degree.; V, Et, 215-16.degree.; V, Pr, 204-5.degree.; V, Bu, 215-16.degree.; V, C₅H₁₁, 214.degree.; V, C₆H₁₃, 194-5.degree.; V, C₁₀H₂₁, 173.degree.. These compds. were tested for activity against polio, adenoviruses, and Toxoplasma gondii. None showed any inhibitory effect on the viruses, but some were effective against toxoplasma in mice. The death-delaying effect of II (R = C₆H₁₃), IV (R = C₅H₁₁), and V (R lower than C₆H₁₃) was nearly equal to that of sulfadiazine or sulfamethazine.

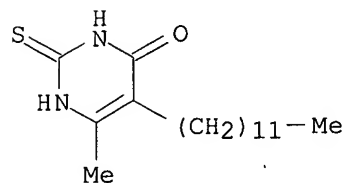
IT 59224-18-9, Uracil, 6-methyl-5-octyl-2-thio- 59224-20-3,
Uracil, 5-decyl-6-methyl-2-thio- 93812-65-8, Uracil,
5-dodecyl-6-methyl-2-thio-
(prepn. of)
RN 59224-18-9 CAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thio- (9CI) (CA
INDEX NAME)



RN 59224-20-3 CAPLUS
CN 4(1H)-Pyrimidinone, 5-decyl-2,3-dihydro-6-methyl-2-thio- (9CI) (CA
INDEX NAME)

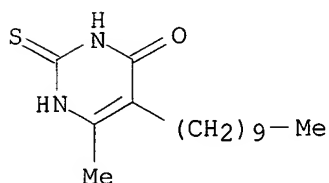


RN 93812-65-8 CAPLUS
CN Uracil, 5-dodecyl-6-methyl-2-thio- (7CI) (CA INDEX NAME)

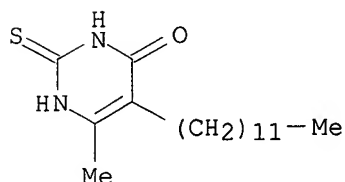


L14 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1963:81563 CAPLUS
 DOCUMENT NUMBER: 58:81563
 ORIGINAL REFERENCE NO.: 58:13969b-c
 TITLE: 5-Alkyl-6-methylthiouracils
 INVENTOR(S): Ueda, Takeo; Kato, Sadatake
 PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd.
 SOURCE: 1 p.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 36008582		19610624	JP	19580324
AB	A mixt. of 12 g. Na, 25 cc. MeOH, 2.7 g. thiourea, and 7.3 g. Et .alpha.-decylacetoacetate is refluxed 10 hrs., evapd., the residue dissolved in H2O, adjusted to pH 4 with AcOH, and the pptd. mass recrystd. from MeOH to give 4.2 g. 5-decyl-6-methyl-2-thiouracil, needles, m. 162-3.degree.. Similarly prepd. is 5-dodecyl-6-methyl-2-thiouracil, needles, m. 150-3.degree. (MeOH). These are useful as remedies for diseases caused by pathogenic virus.				
IT	59224-20-3, Uracil, 5-decyl-6-methyl-2-thio- 93812-65-8, Uracil, 5-dodecyl-6-methyl-2-thio- (prepn. of)				
RN	59224-20-3 CAPLUS				
CN	4(1H)-Pyrimidinone, 5-decyl-2,3-dihydro-6-methyl-2-thioxo- (9CI) (CA INDEX NAME)				

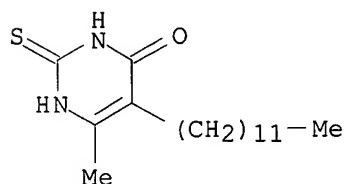


RN 93812-65-8 CAPLUS
 CN Uracil, 5-dodecyl-6-methyl-2-thio- (7CI) (CA INDEX NAME)

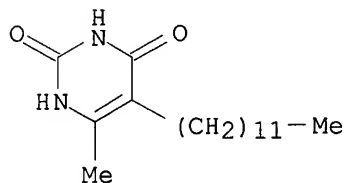


L14 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1962:416927 CAPLUS
 DOCUMENT NUMBER: 57:16927
 ORIGINAL REFERENCE NO.: 57:3445e-g
 TITLE: Syntheses of some heterocyclic compounds with long alkyl side chains and their applications as water-repelling agents for textiles
 AUTHOR(S): Oda, Ryohei; Hayashi, Yoshiyuki
 CORPORATE SOURCE: Univ. Kyoto
 SOURCE: Kogyo Kagaku Zasshi (1961), 64, 1230-3
 CODEN: KGKZA7; ISSN: 0368-5462

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB The following heterocyclic compds. which have long alkyl side chains were synthesized: 2-(.beta.-laurylaminoethyl)-4,6diamino-1,3,5-triazine, .alpha.-laurylimidazolidone, 1-oxo-4-laurylhexahydro-1,3,5-triazine, 1-thioxo-4-laurylhexahydro-1,3,5-triazine, 2,5-dimethyl-N-methyl-N-laurylpyrrolium iodide, 4-methyl-6-lauryluracil, 2-thio-4-methyl-6-lauryluracil, 1-heptadecyl-3,4-dihydroisoquinoline, and 2-undecyl-4-quinazolone. Some of these heterocyclic compds. can be methylolated with HCHO under alk. conditions and give water-repelling effect to cotton fabrics, when applied in the form of emulsion to the fabrics and cured.
 IT 93812-65-8, Uracil, 5-dodecyl-6-methyl-2-thio- 94825-11-3
 , Uracil, 5-dodecyl-6-methyl-
 (prepn. of)
 RN 93812-65-8 CAPLUS
 CN Uracil, 5-dodecyl-6-methyl-2-thio- (7CI) (CA INDEX NAME)

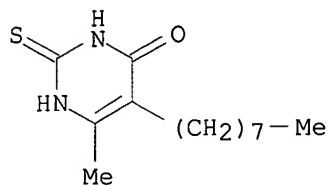


RN 94825-11-3 CAPLUS
 CN Uracil, 5-dodecyl-6-methyl- (7CI) (CA INDEX NAME)

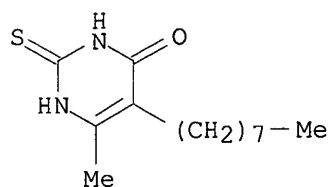


L14 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1950:15848 CAPLUS
 DOCUMENT NUMBER: 44:15848
 ORIGINAL REFERENCE NO.: 44:3156e-g
 TITLE: Studies on the antithyroid and leucopoietic activity of several derivatives of 2-thio-6-methyluracil
 AUTHOR(S): Jurand, Artur; Niwelinski, Jozef
 CORPORATE SOURCE: Univ. Krakow, Pol.
 SOURCE: Bull. intern. acad. polon. sci., Classe med. (1949) 87-101
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB cf. C.A. 43, 2326c. Condensation of thiourea with the corresponding alkyl acetoacetic ester gave the following 5-alkyl-2-thio-6-methyluracils (m.p.): Pr, 213.degree.; (1) Bu, 201.degree.; (2) Am, 183.degree.; heptyl, 184.degree.; octyl, 182.degree.; iso-Pr, 257.5.degree.; (3) iso-Bu, 227.degree.; (4) iso-Am, 216.degree.. The antithyroid and leucocytic activities were compared after oral administration to rabbits. Results on previously unreported compds are: % change in white cell count, Antithyroid activity; 2-thio-6-methyluracil, -28%, +++; (1), -15, ++; (2), 85, ++; (3), 65, ++; (4), 110, +.
 IT 59224-18-9, Uracil, 6-methyl-5-octyl-2-thio-

(prepn. of)
RN 59224-18-9 CAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA
INDEX NAME)



L14 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1949:11549 CAPLUS
DOCUMENT NUMBER: 43:11549
ORIGINAL REFERENCE NO.: 43:2326c-e
TITLE: Effect of 5-alkyl (benzyl) derivatives of
2-thio-4-methyluracil on the thyroid gland and the
bone marrow in rabbits
AUTHOR(S): Jurand, Arthur
SOURCE: Nature (London, United Kingdom) (1948), 162, 896
CODEN: NATUAS; ISSN: 0028-0836
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Derivs. contg. the following radicals were prepd. and tested: (1) Pr, (2)
iso-Pr, (3) heptyl, (4) octyl, (5) benzyl. Results: % change in white
cell count, Antithyroid activity; 2-thio-4-methyluracil, -28, ++++; (1),
-30, +++; (2), +52, +; (3), +64, none; (4), +66, none; (5), +15, +;
IT **59224-18-9**, Uracil, 6-methyl-5-octyl-2-thio-
(effect on bone marrow and thyroid gland)
RN 59224-18-9 CAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-6-methyl-5-octyl-2-thioxo- (9CI) (CA
INDEX NAME)



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